

Kondo effect in a single wall carbon nanotube with pressure inducing pseudogaps[☆]

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Abstract

We are interested to study the Kondo effect present in a system with a T-shape ligation between the single-wall carbon nanotube (SWNT) and a magnetic impurity. The system has studied under pressure and it was observed the opening of the gap in the density of states of the zigzag metallic tube. A tight-binding approximation is used to calculate the SWNT Green's functions. Here we study the disappearance of the Kondo peak as the gap opens and its strong influence on the deformation of the conductance curve. The Kondo effect was considered with the atomic approach with $U \rightarrow \infty$ developed previously. Results of the electronic density of states and curves of the conductance are presented.

Keywords: , Kondo effect, Single wall carbon nanotubes, Peierls distortion, Conductance

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1. The Green's function of the zigzag SWNT

Since 90's decade, when they were discovered, the carbon nanotubes has been receiving attention by great part of the scientific community. With unique characteristics, they present a great potential for applications, since such areas as biomedicine [1, 2, 3, 4, 5] to computer science [6, 7, 8].

The experimental evidence of the carbon nanotubes came in 1991 with imaged multi wall carbon nanotubes (MWNTs) using a transmission electron microscope [9] and in 1993 the first single wall carbon nanotubes (SWNTs) were observed [10, 11].

The structure of a SWNT can be described as a graphene sheet rolled into a cylindrical shape so that the structure is one-dimensional with axial symmetry. We can define the chiral vector \vec{C}_h that is related to the circumference of the tube. The chiral vector can be write as a function of the real space unit vetors \vec{a}_1 and \vec{a}_2 of the hexagonal lattice as $\vec{C}_h = m\vec{a}_1 + n\vec{a}_2$. Here, m and n are the integer indexes that defines the three types of the SWNT: the zigzag ($m = 0, n > 0$), the armchair ($m = n > 0$) and the chiral ($0 < |m| < n$). While the armchair tubes are always metallic, the zigzag tubes are metallic when n is multiple of 3 and semicontuctor otherwise.

It is known that the resistivity of a metal with magnetic impurities diluted increases below a characteristic temperature T_K and this effect is known as the Kondo effect [13]. Recent experiments have observed the Kondo effect in metallic carbon nanotubes [12] and it is interesting to investigated the possibility of occurrence in the proposed carbon based structure. In a previous study, we investigated the Kondo effect considering a SWNT under such a magnetic flux which allows an insulator-metal transition [14]. Now, we use a metallic zigzag SWNT (3,0) to study the interplay between the Kondo effect and the open of the gap when a pressure is applied.

In this paper we apply the atomic model[18] to study the Kondo effect on a zigzag SWNT with a magnetic impurity side-coupled to its surface [19]. In the Fig. 1 we can see a pictorial view of the system that consist in a magnetic impurity laterally coupled to a zigzag nanotube.

The magnetic impurity was modeled by the Impurity Anderson Hamiltonian employing the atomic approach [15, 18] and the Green's function of the tube is calculated analytically, adopting a single π -band tight-binding Hamiltonian [16]. The effect of the hydrostatic pressure is represented by adopting the Peierls distortion[17].

The two-dimensional graphite is naturally a zero-gap semiconductor. This

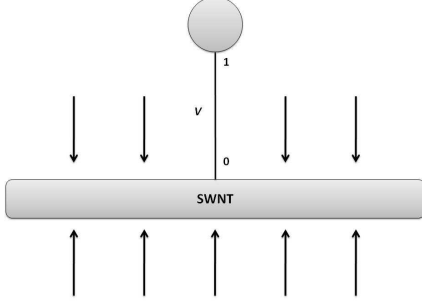


Figure 1: Pictorial view of a carbon nanotube with a magnetic impurity coupled laterally, in the presence of hydrostatic pressure.

occurs because there is an equivalence between C atoms in the unit cell. When a distortion is applied in the lattice, like an out-of-plane deformation, the two atoms become inequivalent. In this case, the position of the atoms is displaced for $+z_0$ and $-z_0$, and an energy gap appears. The width of the gap depends on the electron-phonon coupling α . Therefore, the energy dispersion relation of the distorted zig-zag nanotube $\epsilon_{\pm}(\tilde{k}_x)$ [17], may be written as

$$\epsilon_{\pm}(\tilde{k}_x) = \pm t \sqrt{\Gamma^2 + 1 + 4 \cos(\tilde{q}) \cos(\tilde{k}_x) + 4 \cos^2(\tilde{q})}. \quad (1)$$

with $\tilde{k}_x = \frac{k_x a \sqrt{3}}{2}$, $\tilde{q} = \frac{q\pi}{n}$, $\Gamma = \frac{\alpha z_0}{t}$ and for $-\frac{\pi}{\sqrt{3}} < k_x a < \frac{\pi}{\sqrt{3}}$; $q = 1, \dots, 2n$. D is the tube diameter, a is the lattice parameter, α is the electron-phonon coupling constant and z_0 is the out-of-plane deformation. The out-of-plane deformation produces a result qualitatively similar to the hydrostatic applied to the tube. An energy gap appears with increasing deformation z_0 . Thus, we can study the behavior of the Kondo peak with the opening of the gap, changing only the term distortion of the lattice.

2. Anderson impurity model

The system may be modeled by the Anderson impurity model with infinite Coulomb repulsion ($U \rightarrow \infty$).

The Hamiltonian is given by

$$H = \sum_{\mathbf{k}, \sigma} E_{\mathbf{k}, \sigma} c_{\mathbf{k}, \sigma}^{\dagger} c_{\mathbf{k}, \sigma} + \sum_{\sigma} E_{f, \sigma} X_{f, \sigma \sigma}$$

$$+V \sum_{\mathbf{k},\sigma} \left(X_{f,0\sigma}^\dagger c_{\mathbf{k},\sigma} + c_{\mathbf{k},\sigma}^\dagger X_{f,0\sigma} \right), \quad (2)$$

where the first term represents the conduction electrons (c -electrons) here represented by carbon nanotube conduction band, the second describes the Anderson impurity characterized by a localized f level $E_{f,\sigma}$, (where f indicates localized electrons at the impurity site) and the last one corresponds to the interaction between the c -electrons of the carbon nanotube and the impurity. For simplicity we consider a constant hybridization V . Hubbard operators [20] are employed to project out the double occupation state $|f, 2\rangle$, from the local states on the impurity. The identity decomposition in the reduced space of local states at the impurity is given by $X_{f,00} + X_{f,\sigma\sigma} + X_{f,\bar{\sigma}\bar{\sigma}} = I$, where $\bar{\sigma} = -\sigma$, and the three $X_{f,aa}$ are the projectors into the states $|f, a\rangle$. The occupation numbers on the impurity $n_{f,a} = \langle X_{f,aa} \rangle$ should then satisfy the “completeness” relation

$$n_{f,0} + n_{f,\sigma} + n_{f,\bar{\sigma}} = 1. \quad (3)$$

3. Atomic model

To obtain the exact f Green function $G_{ff,\sigma}(\mathbf{j}_i, z)$ in real space for the impurity at site \mathbf{j}_i , one follows a procedure similar to the one used in [21] within the chain approximation. The exact GF $G_{ff,\sigma}(z)$ is then given by replacing the bare cumulant $M_{2,\sigma}^0(z) = -D_\sigma^0/(z - \varepsilon_f)$ by the effective cumulant $M_{2,\sigma}^{eff}(z)$ at all the filled vertices of the chain diagrams in [21]. The exact GF for the f electron is then written as

$$G_{ff,\sigma}(z) = \frac{M_{2,\sigma}^{eff}(z)}{1 - M_{2,\sigma}^{eff}(z) |V|^2 \sum_{\mathbf{k}} G_{c,\sigma}^o(\mathbf{k}, z)}. \quad (4)$$

The exact atomic f Green function ($G_{ff,\sigma}^{at}(z)$) is calculated exactly in [18] and has the same form of Eq.(4). We can write as

$$G_{ff,\sigma}^{at}(z) = \frac{M_{2,\sigma}^{at}(z)}{1 - M_{2,\sigma}^{at}(z) |V|^2 G_{c,\sigma}^o(\varepsilon_q, z)}, \quad (5)$$

where $G_{c,\sigma}^o(z) = -1/(z - \varepsilon_q)$ is the Green function of the conduction electrons with energy ε_q of the atomic system. From this equation we then obtain an explicit expression for $M_{2,\sigma}^{at}(z)$ in terms of $G_{ff,\sigma}^{at}(z)$

$$M_{2,\sigma}^{at}(z) = \frac{G_{ff,\sigma}^{at}(z)}{1 + G_{ff,\sigma}^{at}(z) |V|^2 G_{c,\sigma}^o(\varepsilon_q, z)}. \quad (6)$$

The atomic approximation consists in substituting $M_{2,\sigma}^{eff}(z)$ in Eq.(4) by the approximate $M_{2,\sigma}^{at}(z)$ given by Eq.(6). The local Green function for the impurity is

$$G_{ff,\sigma}(z) = \frac{M_{2,\sigma}^{at}(z)}{1 - M_{2,\sigma}^{at}(z) |\Delta|^2 G_{jj,\sigma}^o(z)}, \quad (7)$$

where we replace V^2 by Δ^2 to decrease the contribution of the c -electrons, whose effect is overestimated by concentrating them at a single energy level. Here ($\Delta = \pi V^2/2D$) is the Anderson parameter and is on the order of the Kondo peak's width.

The Green function of the pure zigzag carbon nanotube $G_{jj,\sigma}^o(z)$ is obtained analitically [22] employing the tight-binding approximation. In the case of the zigzag carbon nanotube $(n, 0)$, the k_y is quantized.

$$k_y = \frac{2\pi l}{an} \quad (8)$$

where $l = 1, n$. The integration is made on the k_x and the limits range from $-\frac{\pi}{a\sqrt{3}}$ to $\frac{\pi}{a\sqrt{3}}$. We can write de Green function as

$$G_{jj',\sigma}^o(z) = \frac{1}{n} \sum_l \frac{a\sqrt{3}}{2\pi} \int_{-\frac{\pi}{a\sqrt{3}}}^{\frac{\pi}{a\sqrt{3}}} dk_x \frac{ze^{i\vec{k} \cdot (\vec{R}_j^\bullet - \vec{R}_{j'}^\bullet)}}{z^2 - \epsilon_+^2(\tilde{k}_x)}, \quad (9)$$

where $\epsilon_+^2(\tilde{k}_x)$ is given by Eq.(1) and \vec{R}_j^\bullet and $\vec{R}_{j'}^\bullet$ are the position vectors of the site j and j' , respectively.

One still has to decide what value of ε_q should be taken. As the most important region of the conduction electrons is the Fermi energy, we shall use $\varepsilon_q = \mu - \delta E_0$, leaving the freedom of small changes δE_0 to adjust the results in such a way that the completeness relation given by Eq.(3) is satisfied.

4. Results

We are interested to describe the magnetic impurity side-coupled to a metallic zigzag (3, 0) SWNT. To low temperatures and bias voltage the electronic transport is coherent and the conductance is calculated by Landauer

equation[23]

$$G = \frac{2e^2}{\hbar} \int \left(-\frac{\partial n_F}{\partial \omega} \right) S(\omega) d\omega, \quad (10)$$

with n_F is the Fermi function and $S(\omega)$ is the transmission probability of an electron with energy $\hbar\omega$ and is given by

$$S(\omega) = \gamma^2 |G_{00}^\sigma|^2, \quad (11)$$

where γ corresponds to the coupling strength of the site 0 to the tube (which is proportional to the kinetic energy of the electrons in the site 0 of the tube). G_{00}^σ is the Green function at the site 0 and can be calculated by the Dyson equation, with the hybridization operator $\hat{V} = |0\rangle\tilde{V}\langle 1| + |1\rangle\tilde{V}\langle 0|$ (see Fig. 1). The hybridization \tilde{V} is the energy that join the ballistic channel to impurity. In this work we use $\tilde{V} = 3V$, where V is the hybridization of the atomic case (sec.3).

The dressed Green's functions G_{00} can be written in terms of the dressed localized Green's functions G_{11} of the magnetic impurity, and in terms of the undressed Green's functions g_{00} of the conduction electrons of the SWNT.

$$G_{00}^\sigma = g_{00}^\sigma (1 + g_{00}^\sigma \tilde{V}^2 G_{11}^\sigma), \quad (12)$$

where g_{00}^σ is the Green's function of the SWNT given by the Eq.(9) and the G_{11}^σ is given by the Eq.(7).

In the Fig. 2 we show the density of states (DOS) of the system for $E_f = -5.0\Delta$ and $T = 0.01\Delta$, without pressure applied ($\Gamma = 0$). This situation correspond to Kondo regime, which is marked by the presence of the Kondo peak. On the right detail of the figure we show the DOS ρ_c of the conduction electrons of the zigzag (3, 0) SWNT, where $\rho_c = -\frac{1}{\pi}\text{Im}(g_{00})$. On the left detail of the figure we can see the Kondo peak on the chemical potential $\mu = 0$. The wider Peak is the resonance over the localized level $E_f = -5.0\Delta$.

In the set of Fig. 3 - Fig. 5 we vary the parameter (Γ) while all the others parameters of the previous case are fixed. In the Fig. 3 and Fig. 4 the parameter relatad with the pressure is used with the values $\Gamma = 0.0005$ and $\Gamma = 0.0012$ respectively, and a pseudogap is forming on the conduction band of the SWNT. We can see that the Kondo peak height increases in a subtle way and the curves for these small values of $\Gamma = 0.0005$ and $\Gamma = 0.0012$ are

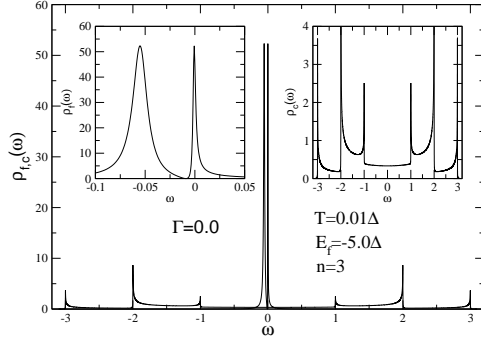


Figure 2: Density of states of a (3,0) SWNT, $\Gamma = 0.0$, temperature $T = 0.01\Delta$, and the localized f level at $E_f = -5.0\Delta$ in the Kondo regime.

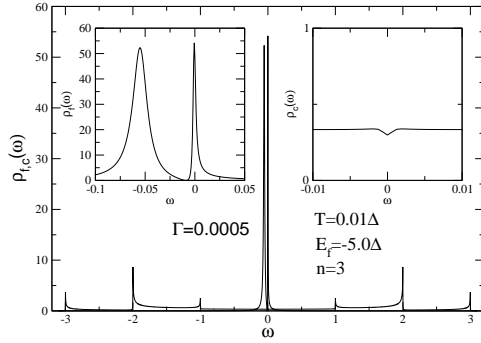


Figure 3: Density of states of a (3,0) SWNT, $\Gamma = 0.0005$, temperature $T = 0.01\Delta$, and the localized f level at $E_f = -5.0\Delta$ in the Kondo regime.

very close to the case without pressure $\Gamma = 0$, ie, the Kondo effect is still acting.

In the Fig. 5 we use $\Gamma = 0.01$, which is the extreme value for high pressure. Here the gap is fully formed and the Kondo effect doesn't exist anymore. The Kondo resonance was split up and relocated of the chemical potential and the relation of completeness is not satisfied.

The Fig. 6 represent the density of states localized at the chemical potential μ , that is $\rho(\omega = \mu)$ for $\mu = 0$ as function of the parameter Γ . The system

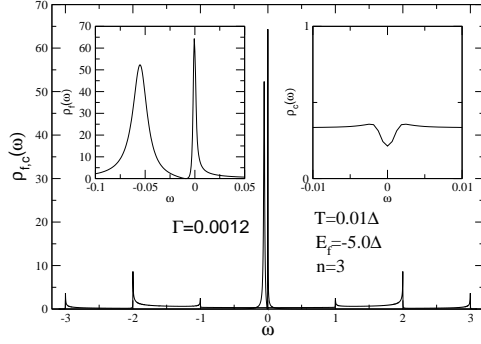


Figure 4: Density of states of a (3,0) SWNT, $\Gamma = 0.0012$, temperature $T = 0.01\Delta$, and the localized f level at $E_f = -5.0\Delta$ in the Kondo regime.

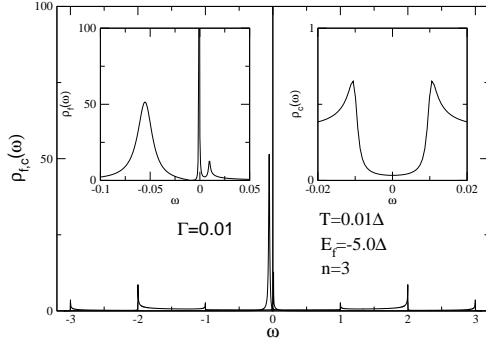


Figure 5: Density of states of a (3,0) SWNT, $\Gamma = 0.01$, temperature $T = 0.01\Delta$, and the localized f level at $E_f = -5.0\Delta$ in the Kondo regime.

is kept in the Kondo regime for $E_f = -5\Delta$ and $T = 0.01\Delta$. The figure indicates the gradual formation of the gap, which causes the increase of the Kondo peak until a certain value of $\Gamma \cong 0.0025$. The increase in height of the Kondo peak produces a narrowing of its width, which indicates a decrease in the Kondo temperature T_K as the pressure is applied. For large values of applied pressure ($\Gamma > 0.0025$), the gap is fully formed and the Kondo peak is destroyed. The system now behaves like a semiconductor.

The Fig. 7 represent the conductance as fuction of the localized level of

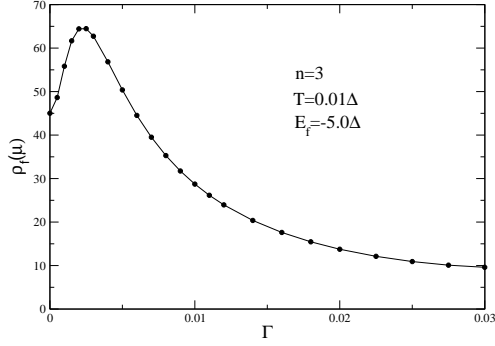


Figure 6: Density of states localized at the chemical potential $\mu = 0.0\Delta$ in function of Γ for $T = 0.01\Delta$ and the localized f level at $E_f = -5.0\Delta$ in the Kondo regime.

the impurity E_f , for different values of Γ . For small values of Γ , the Kondo effect is present and the conductance is suppressed only in the Kondo region. As the value of Γ is increased, the gap opens and the Kondo effect disappears. For the value of $\Gamma = 0.01$, the gap is fully open and the conductance goes to zero, indicating that the Kondo effect is not present and that the system behaves like a semiconductor.

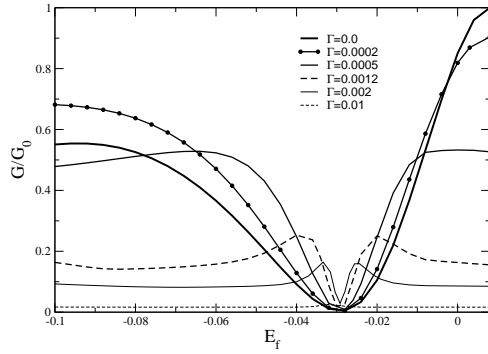


Figure 7: Conductance as a function of E_F for different values of Γ . The temperature $T = 0.01\Delta$, and the localized f level at $E_f = -5.0\Delta$ in the Kondo regime.

5. Conclusions

In this work we have employed the atomic approach [18] to study the disappearance of the Kondo effect when the hydrostatic pressure induces an metal-insulator transition in a metallic SWNT. In order to reproduce the effect of hydrostatic pressure applied to the nanotube, we used the out-of-plane deformation, which produces qualitatively similar results. Results of the electronic density of states, characterizing the structure of the Kondo peak at the chemical potential were presented. We show that increased pressure increases the height of the Kondo peak and, consequently, its width decreases, indicating a decrease in the Kondo temperature. We also present the curve of conductance that was calculated for different values of Γ and the results presented are consistent with previous studies in the region of zero pressure. These studies support a more detailed investigation of the effects of the strong correlation in nanostructured systems in the presence of external agents, like applied pressure or electric/magnetic fields.

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